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Title:	Natural Convection in a Storage Container: Coupling Abaqus to a Surrogate Model
Author(s):	Fister, Matthew Wood
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Natural Convection in a Storage Container

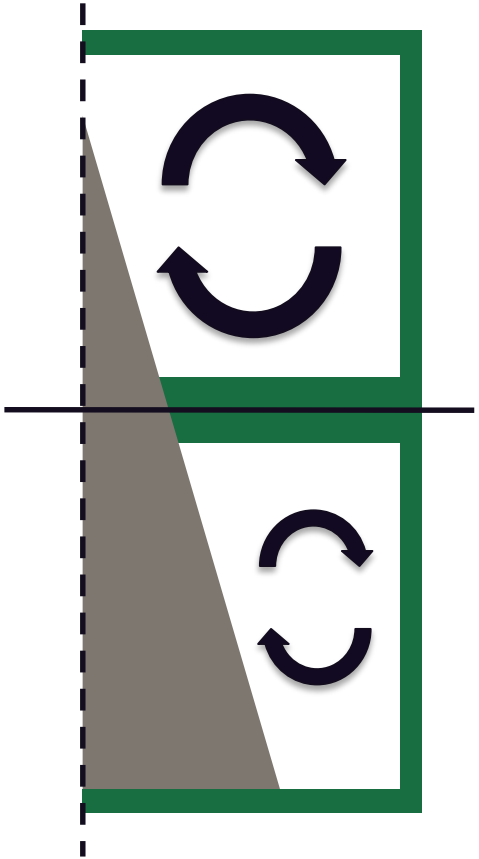
Coupling Abaqus to a Surrogate Model

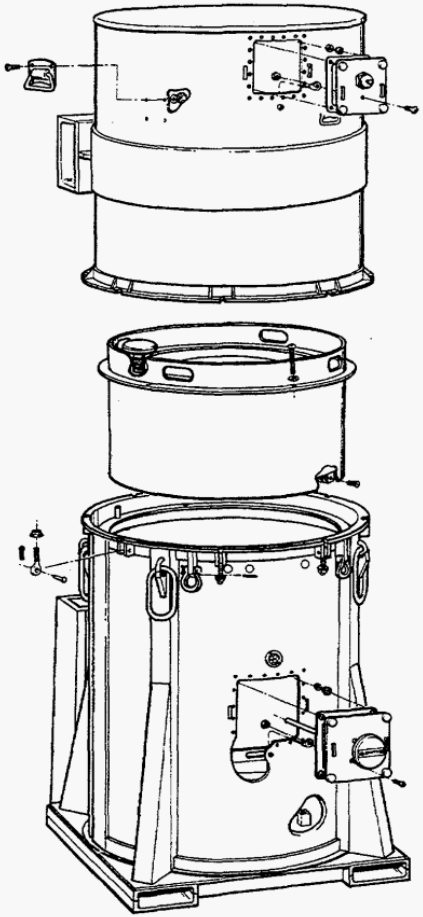
Matt Fister

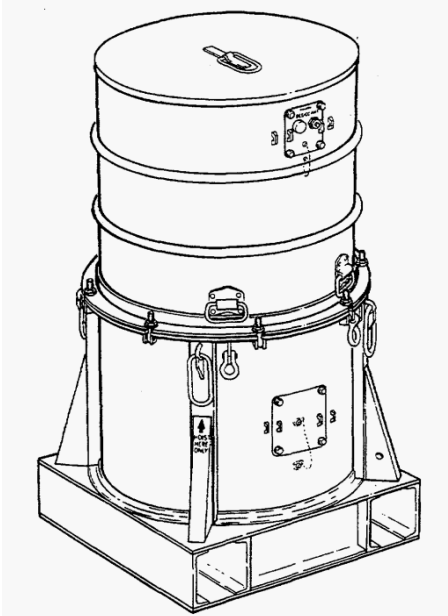
September 4, 2019

NNSA
National Nuclear Security Administration
Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Internal heat source causes natural convection in storage containers.







SANDIA REPORT

SAND97–8017 • UC–700
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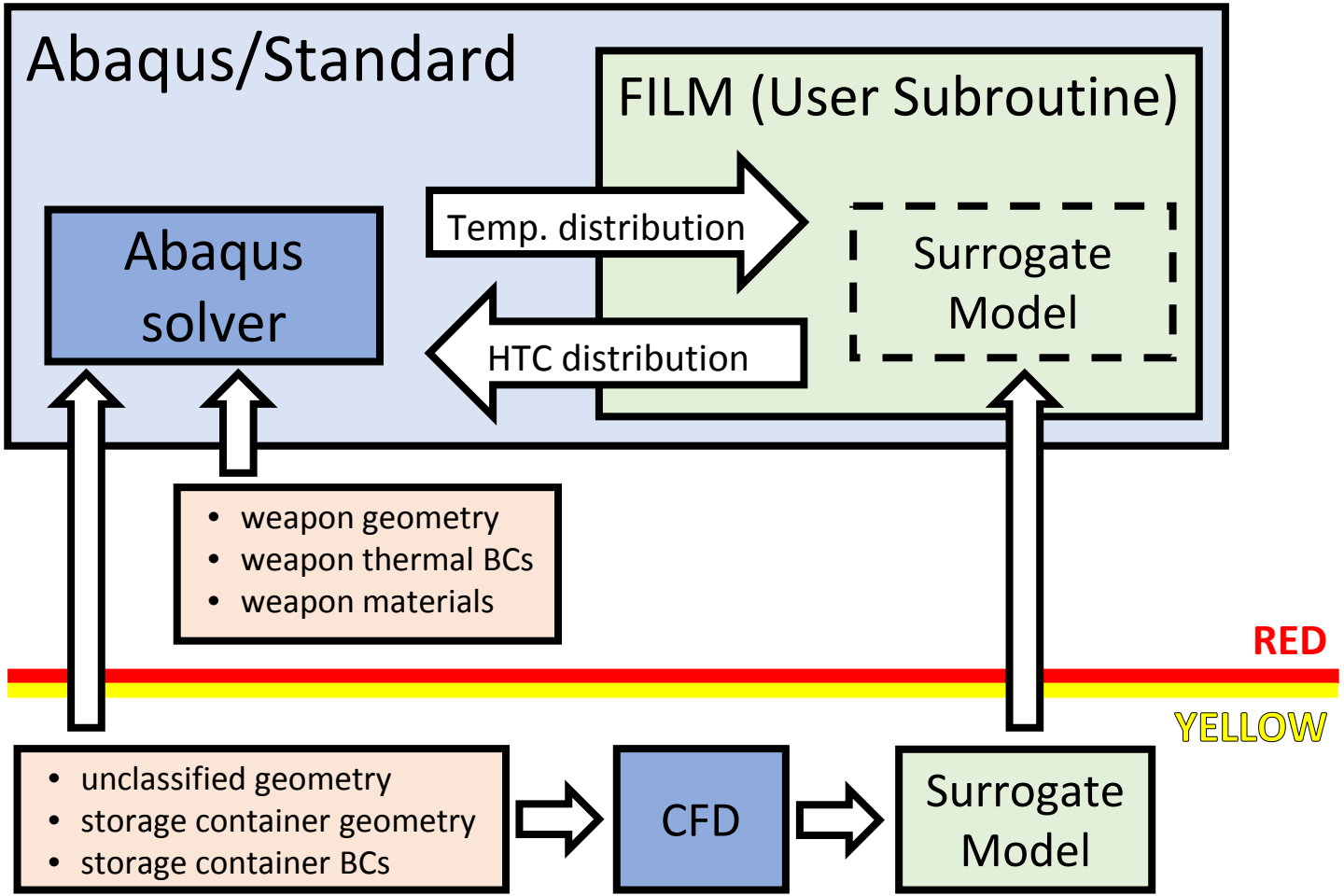
Weapon Container Catalog

Volumes 1 & 2

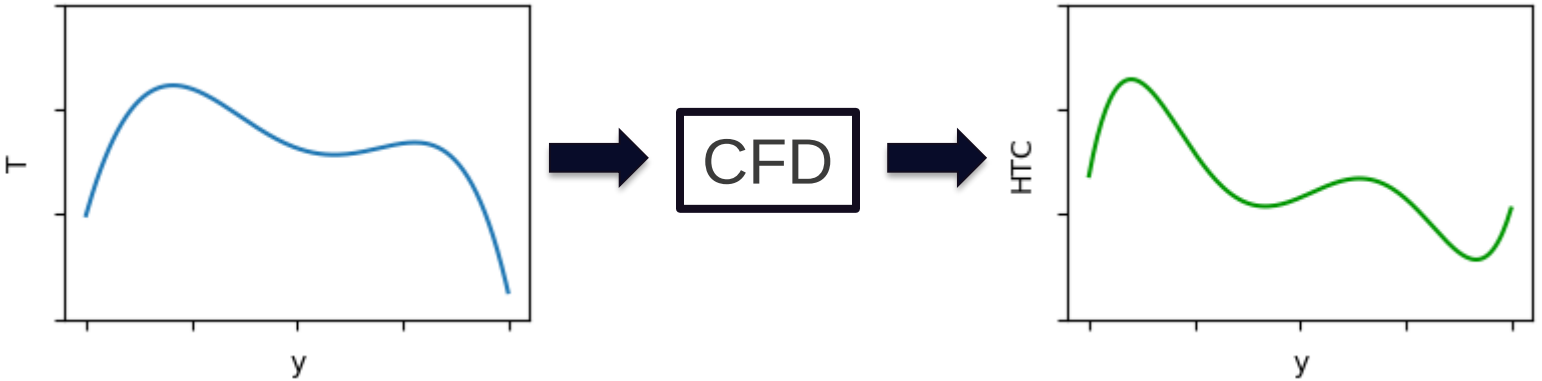
How can we add convection to existing FE model?

- 3DExperience
  - no licenses; E-13 said no
- Couple Abaqus with CFD code
  - communication at each increment
    - Abaqus supports file I/O for this purpose; does CFD code?
    - some assembly required (file formatting, timing, etc.)
    - requires concurrent installations and licensing for both codes
      - for reference, I'm running Fuego out of Temo's /scratch on Hamming!
  - communication at each job
    - requires multiple Abaqus runs
    - only works well if few iterations are required (i.e. not strongly coupled physics)
    - some assembly required
- Or…

We could couple Abaqus to a surrogate model.

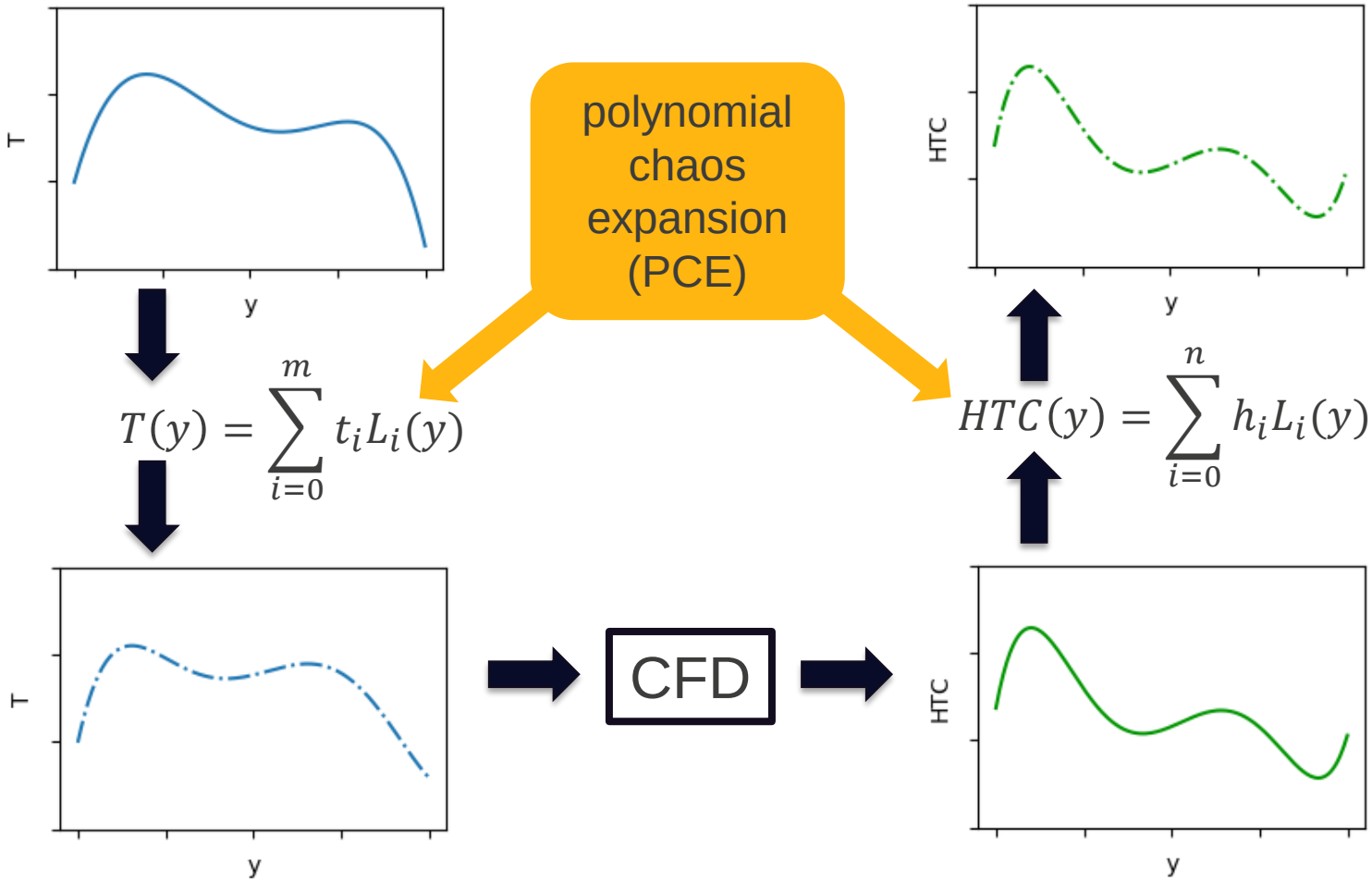


How do we build the surrogate model?

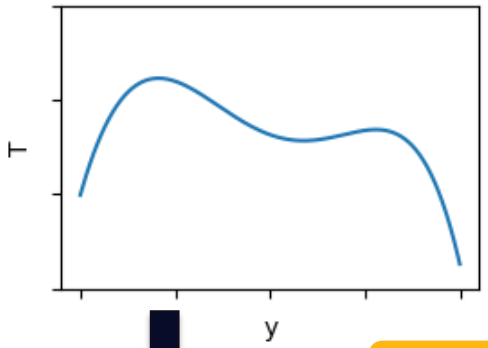


We need scalar inputs and outputs!*

How do we build the surrogate model?

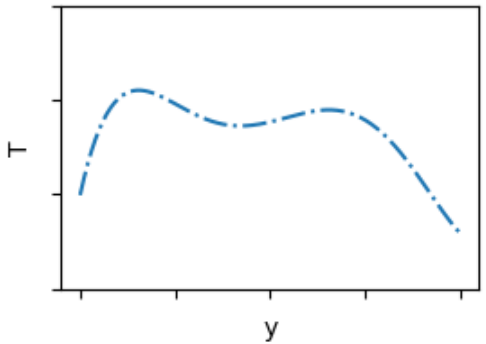


How do we build the surrogate model?

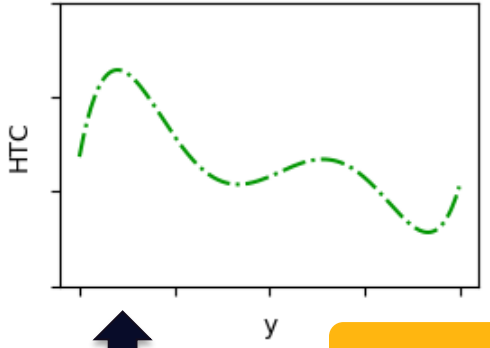


$$T(y) = \sum_{i=0}^{m} t_i L_i(y)$$

scalar inputs

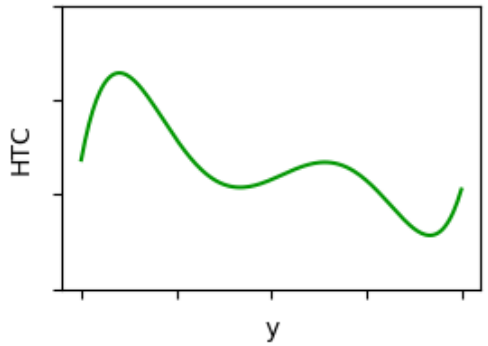


CFD



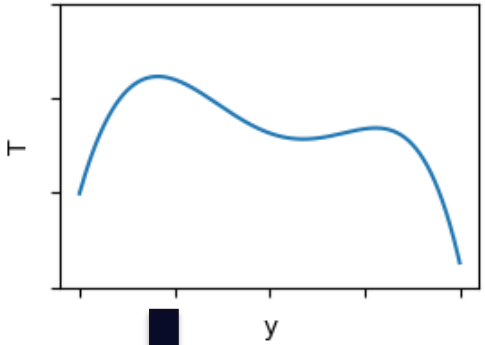
$$HTC(y) = \sum_{i=0}^{n} h_i L_i(y)$$

scalar outputs



Surrogate modeling has its limitations.

Does our input space encompass the T distributions Abaqus will give us?

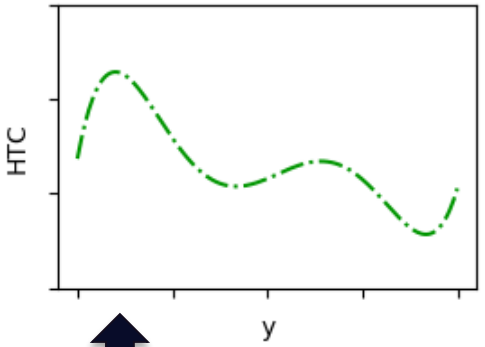


$$T(y) = \sum_{i=0}^{m} t_i L_i(y)$$

How well does PCE match the T distribution from Abaqus?

How well does the surrogate model match the CFD calculations?

Surrogate model

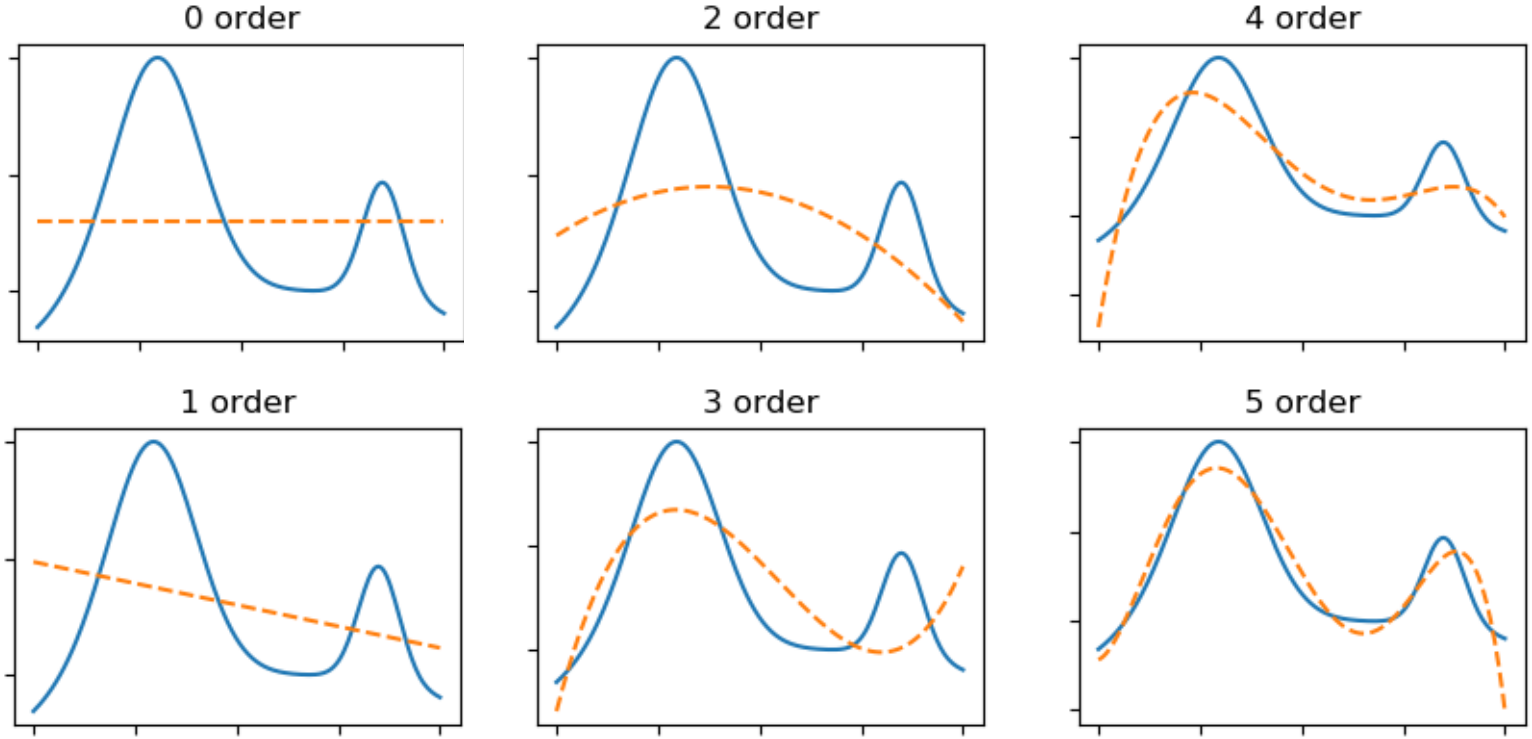


$$HTC(y) = \sum_{i=0}^{n} h_i L_i(y)$$

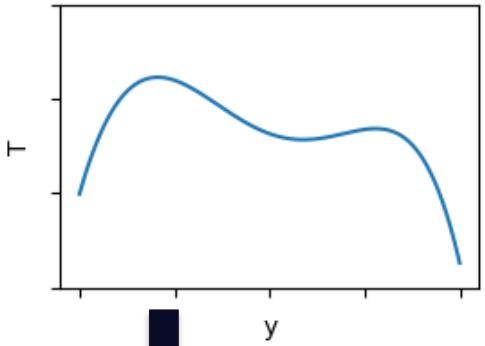
How well does PCE match the HTC distribution from CFD?

How do we choose the surrogate's input parameter space?

- # of dimensions in input domain determines what shape T distribution we can handle



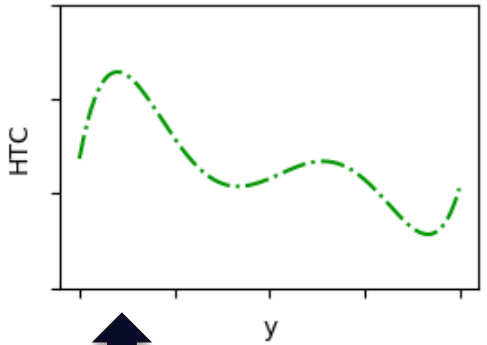
How do we choose the surrogate model form?



$$T(y) = \sum_{i=0}^{m} t_i L_i(y)$$

How simple is the relationship between t_i and h_i?

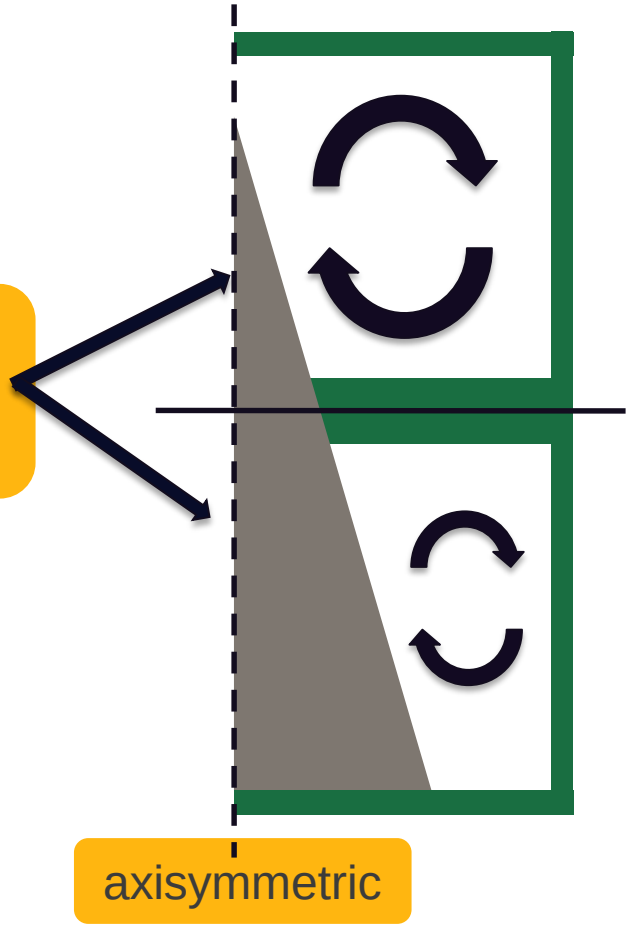
Surrogate model



$$HTC(y) = \sum_{i=0}^{n} h_i L_i(y)$$

Would the relationship be simpler if we used different decompositions?

Surrogate model form depends on the CFD model.



"upper chamber" and "lower chamber" modeled separately

axisymmetric

container
- isothermal, 300 K
- no-slip

air
- sea-level
- Boussinesq

unclassified geometry
- constant temp. (hot)
- non-uniform temp.
- no-slip

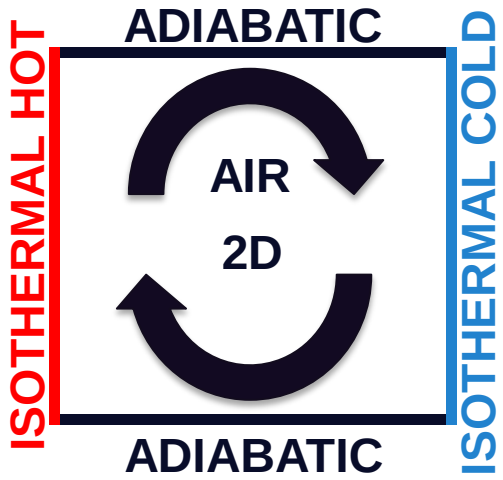
What CFD software is available to E-13?

- Ansys Fluent
  - widely used, commercial software
  - detailed documentation, lots of examples, large community
  - not E-13 software
  - previously ran on E-1's 20-core computer via RDP
- Sierra Fuego
  - not widely used (here)
  - "documentation" is a half-complete, auto-generated API
  - also not E-13 software
  - currently running from Temo's /scratch on yellow Hamming
  - requires no licenses, can run on Hamming via SSH

Will Fuego work for low ΔT problems?

- Fuego was created for modeling fires
  - natural convection, but much higher thermal gradients
- Our application has temperature differences < 10 K
- Abundant literature on natural convection provides ways of "verifying" Fuego for our problem
  - experimental data and numerical solutions

Verification Problem #1



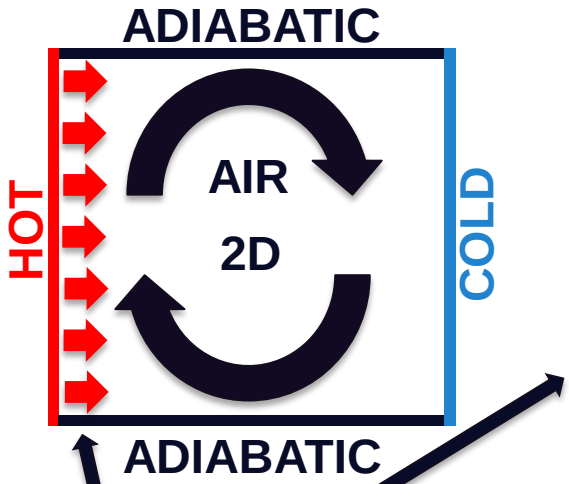
$$\mathrm{Nu} = 0.18\left(\frac{\mathrm{Pr}}{0.2+\mathrm{Pr}}\mathrm{Ra_H}\right)^{0.29}\left(\frac{\mathrm{L}}{\mathrm{H}}\right)^{-0.13}$$

Non-dimensional numbers in natural convection.

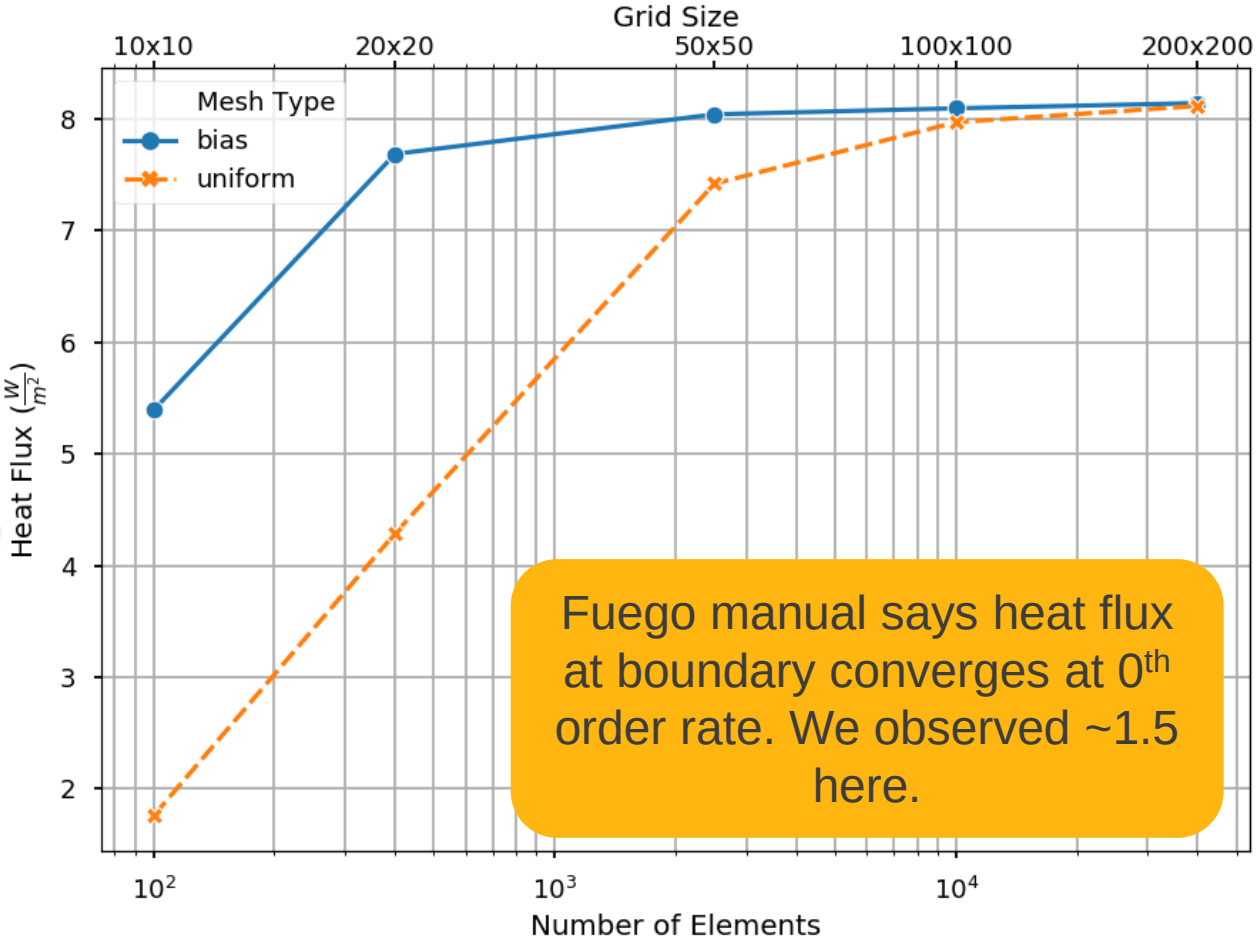
- Ra – Rayleigh number
  - characterizes flow regime (laminar vs turbulent)
  - Gr * Pr
  - x-axis for lots of empirical natural convection relationships
- Gr – Grashof number
  - ratio of buoyancy forces to viscous forces
  - Reynolds number for natural convection
- Pr – Prandtl number
  - ratio of thermal to velocity boundary layer thicknesses
  - material property (~0.7 for air)
- Nu – Nusselt number
  - ratio of convective to conductive heat transfer

Good mesh convergence for Verification Problem #1.

Verification Problem #1



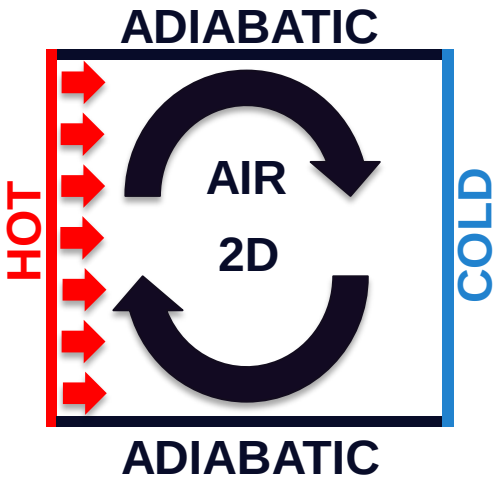
Heat Flux through left (hot) wall



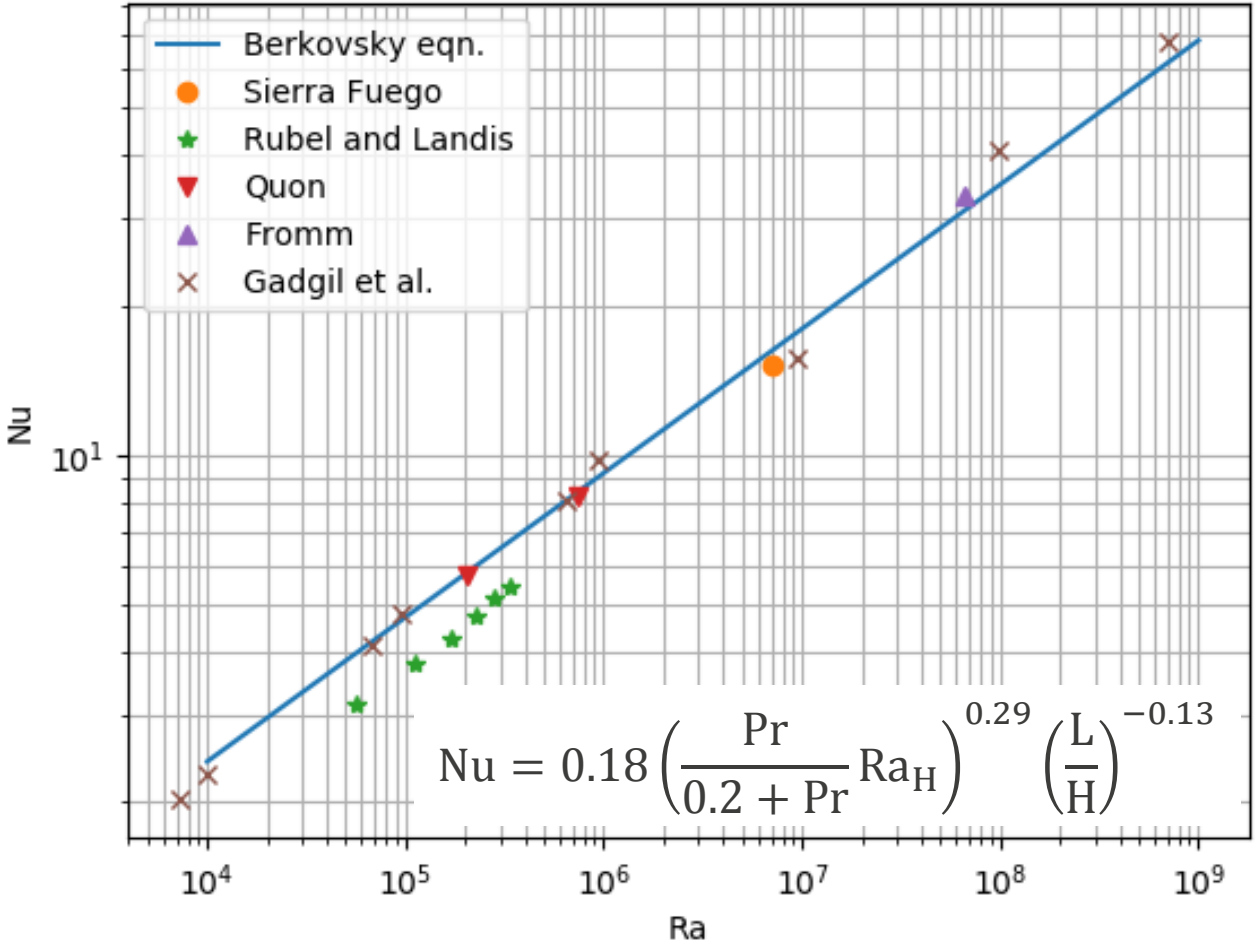
Fuego manual says heat flux at boundary converges at 0th order rate. We observed ~1.5 here.

Verification Problem #1 solution agrees well with published results.

Verification Problem #1

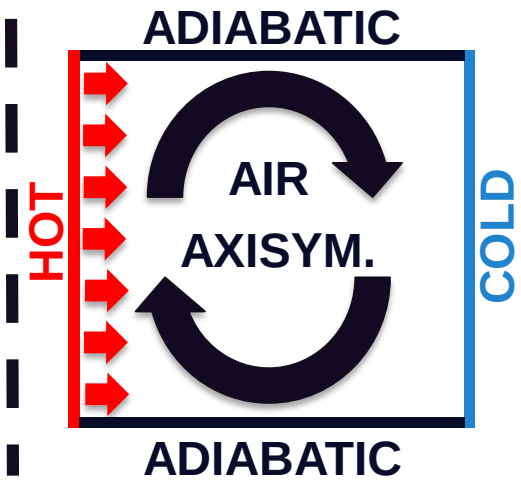


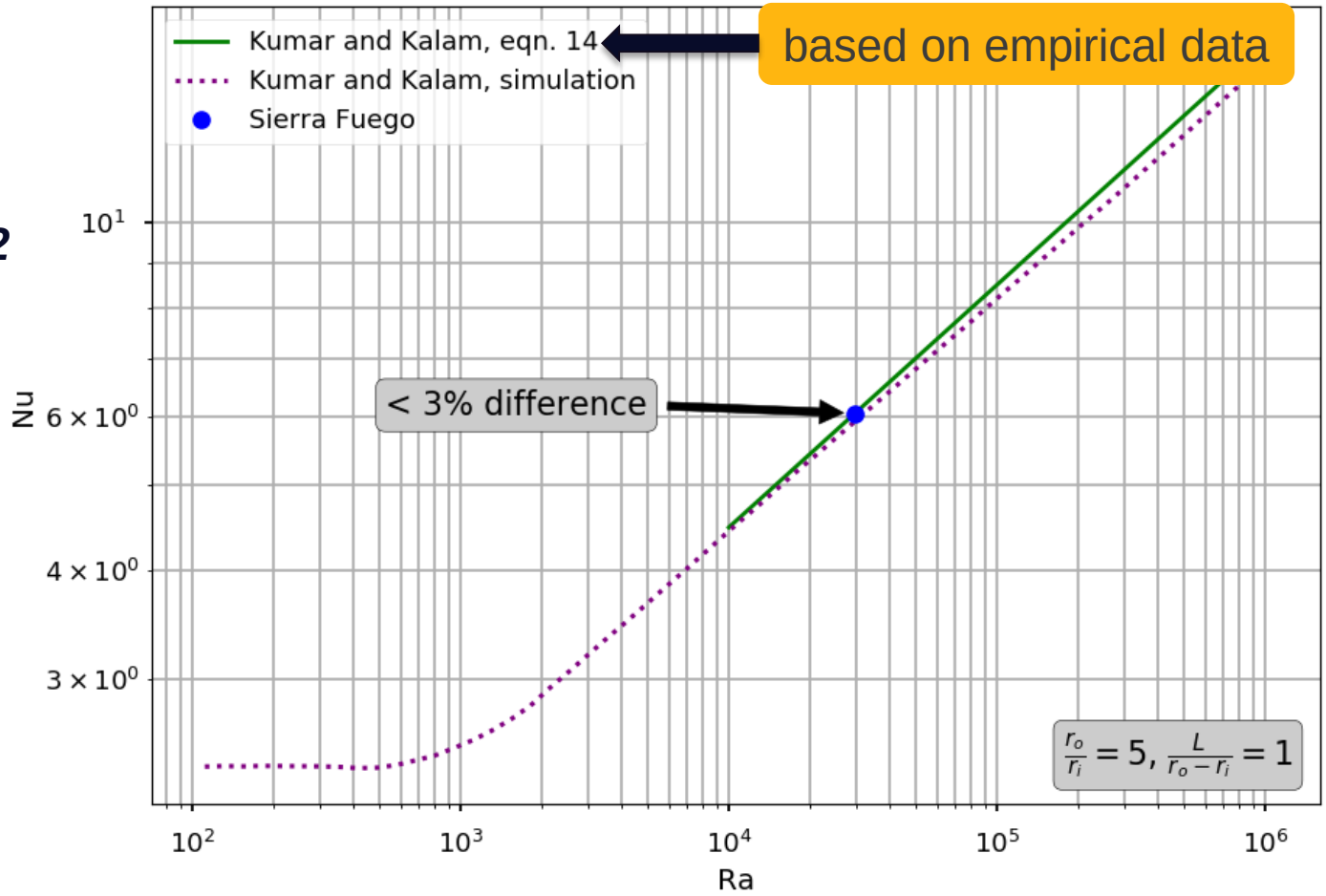
Streamlines and isothermal contours qualitatively match published results as well.



Fuego matches published results for Verification Problem #2.

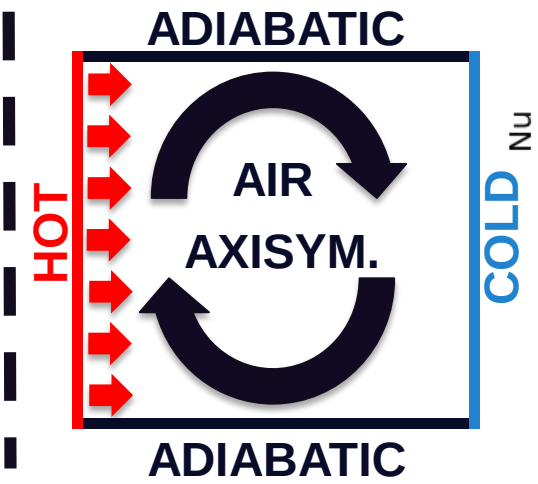
Verification Problem #2

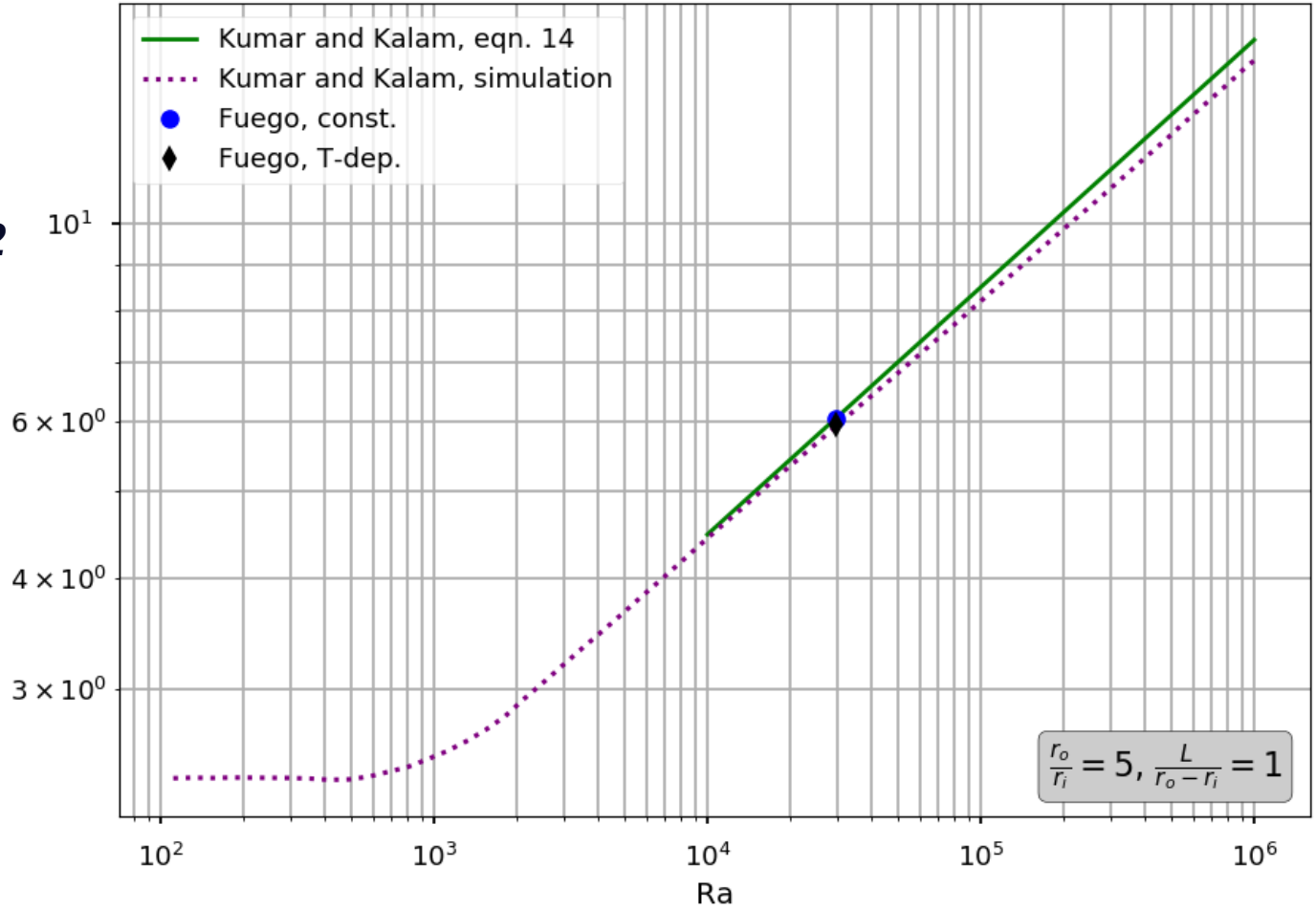




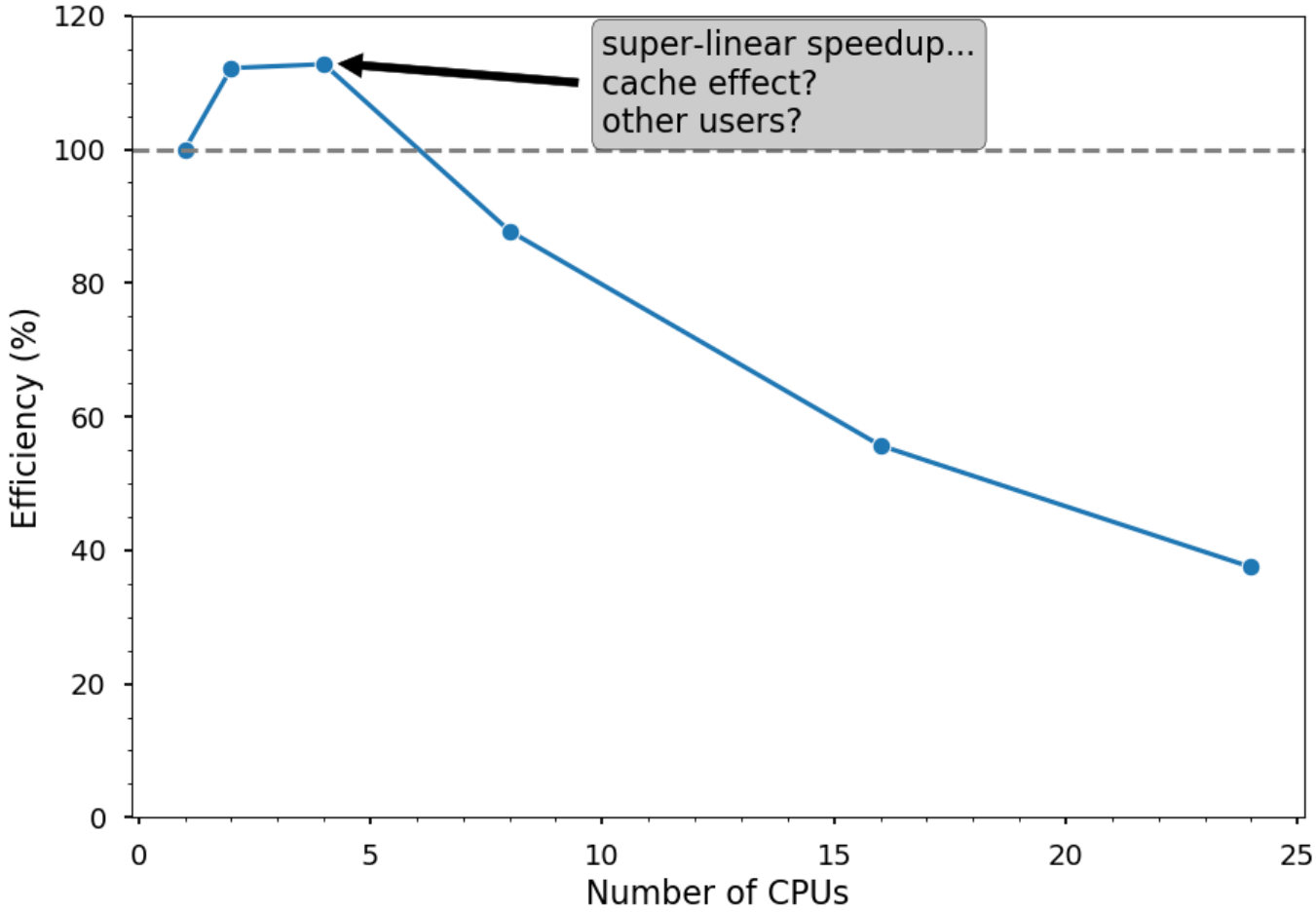
Temperature-dependent air properties don't matter for our problem.

Verification Problem #2

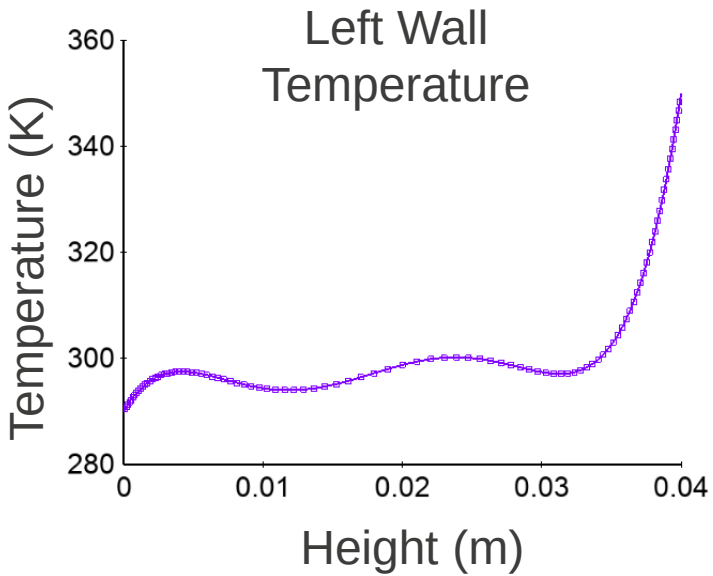


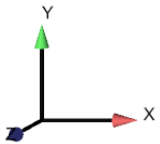


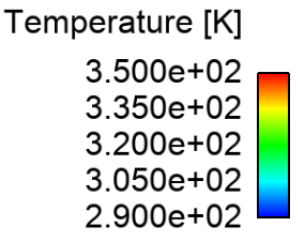
Fuego model scales efficiently to at least 4 cores.



It’s easy to apply PCE temperature distribution in Fuego.





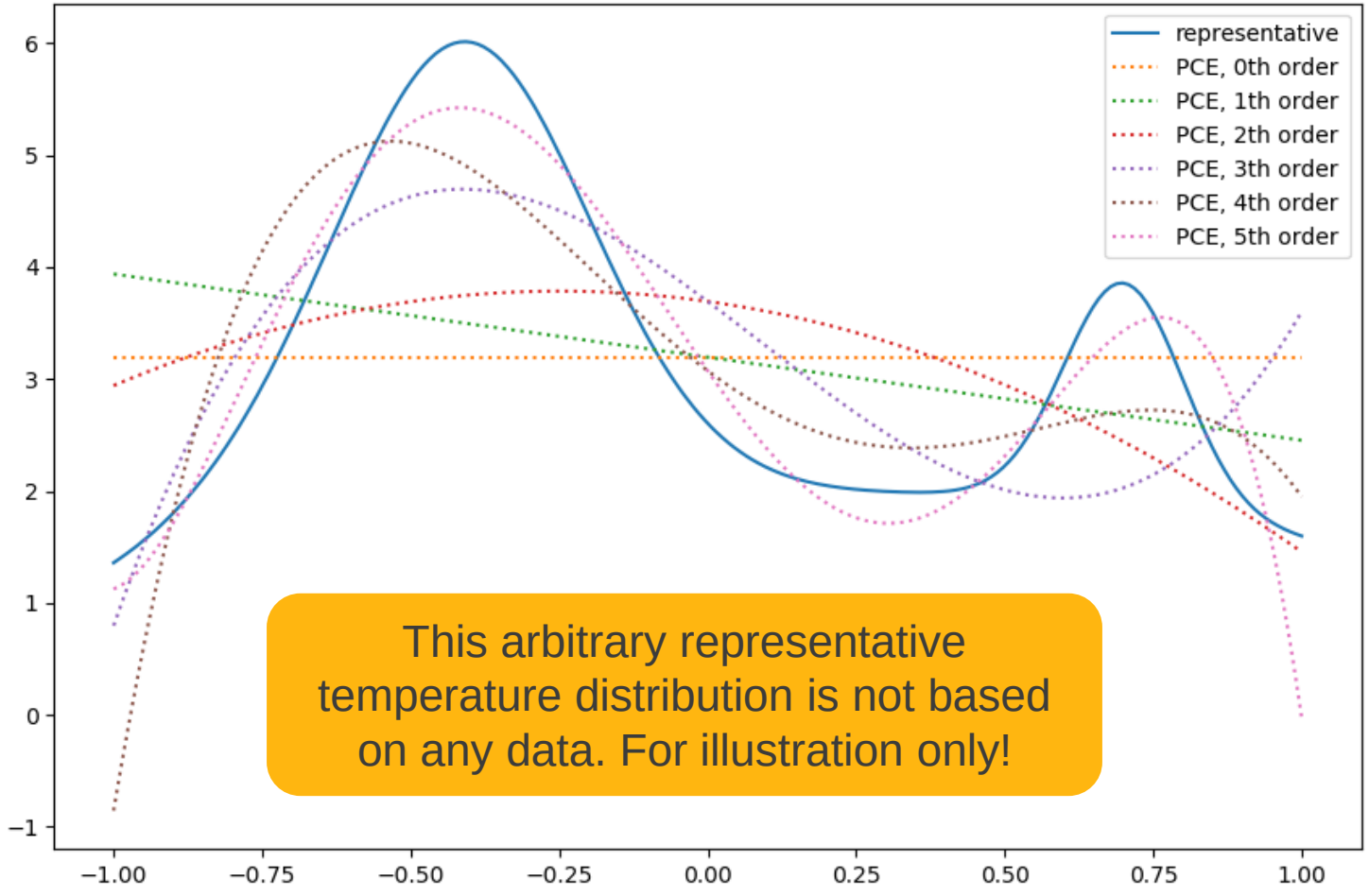


There are 2 main questions regarding the surrogate model.

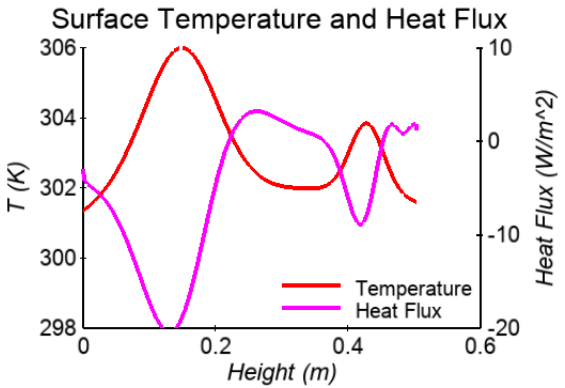
1. How big should the input space be?
   - i.e. how accurately do we need to model the temperature distribution?

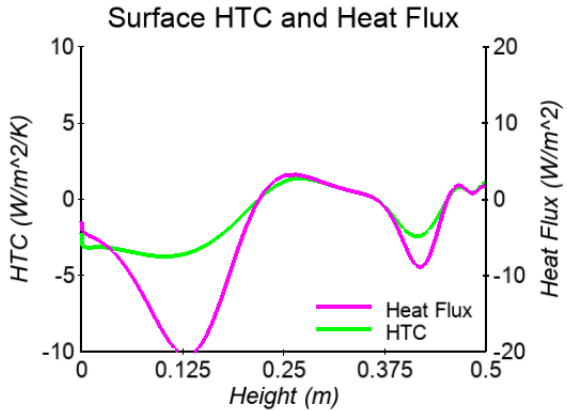
2. Can a surrogate model accurately relate our inputs to our outputs?
   - inputs: PCE coefficients for temperature
   - outputs: PCE coefficients for HTC

“Good enough” depends on the FE model’s sensitivity to the PCE.

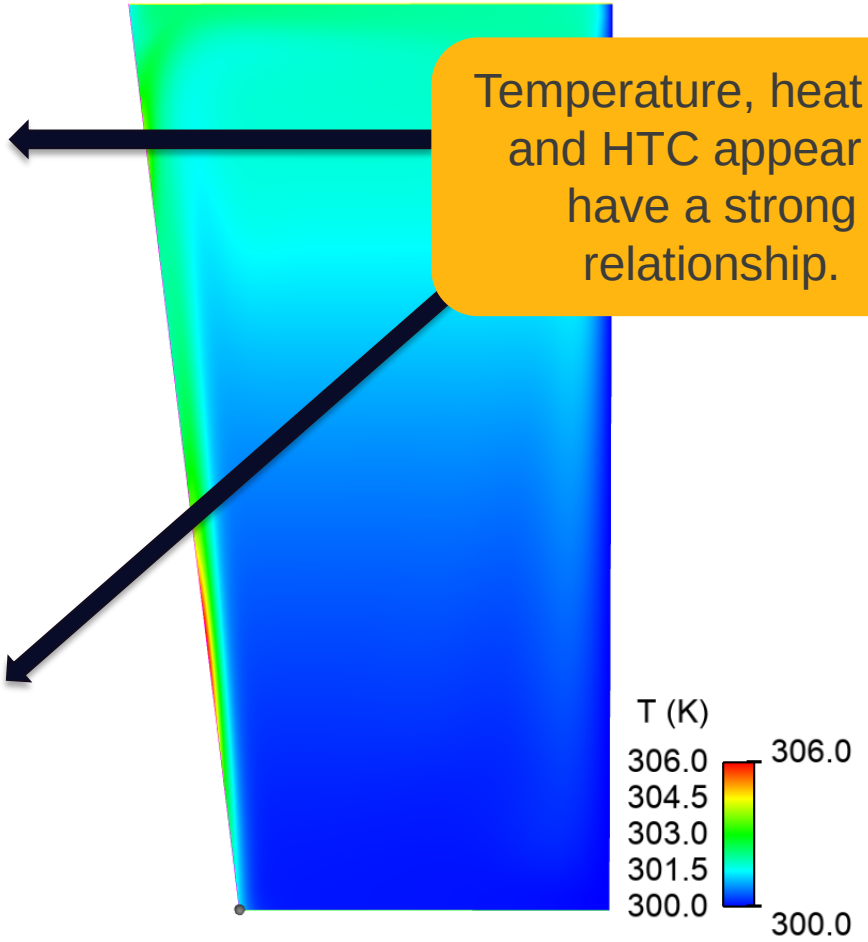


CFD results using example temperature distribution.



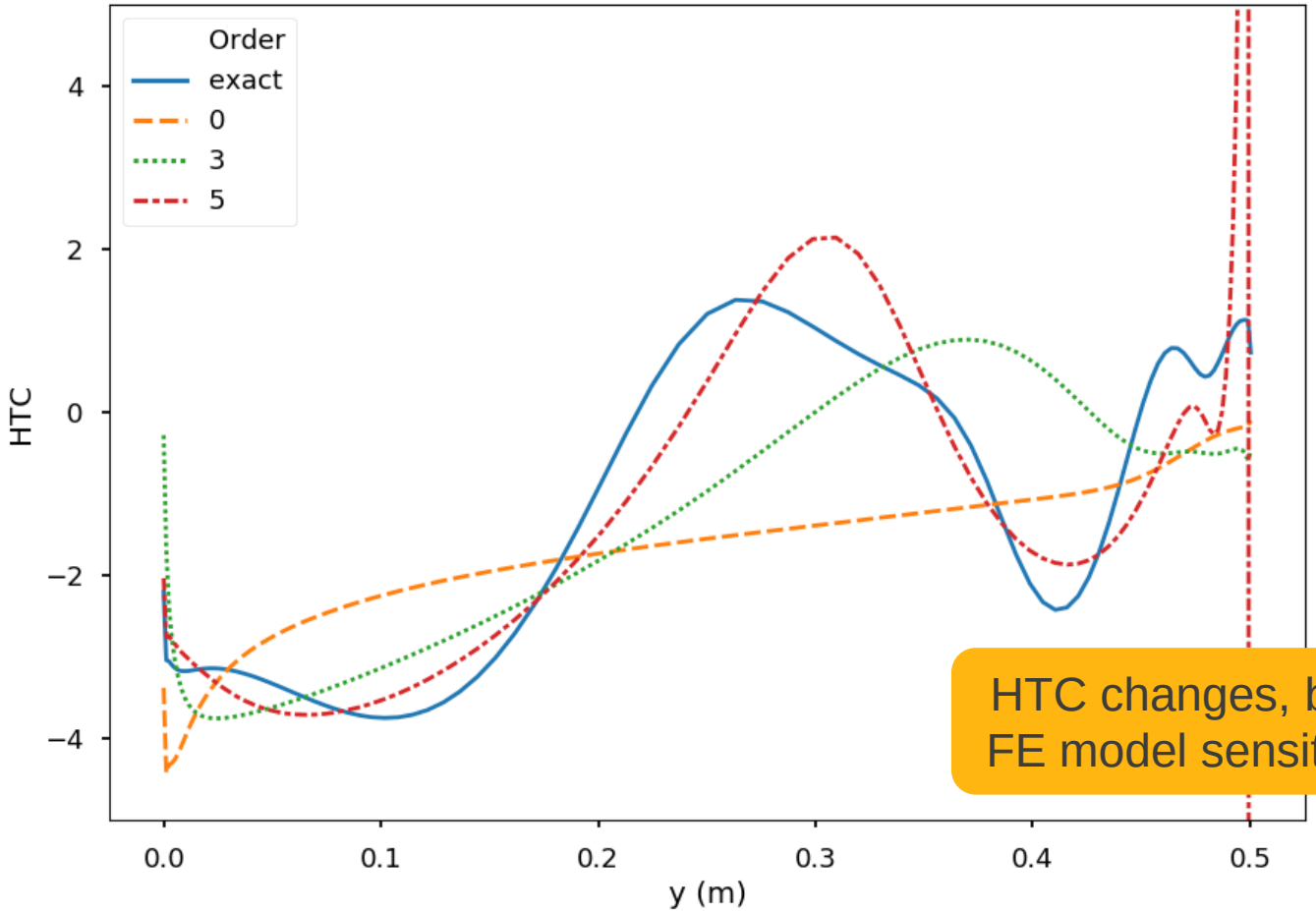


Heat Transfer Rate (W): -3.061



Temperature, heat flux and HTC appear to have a strong relationship.

HTC is sensitive to the temperature PCE accuracy.



HTC changes, but is the FE model sensitive to it?

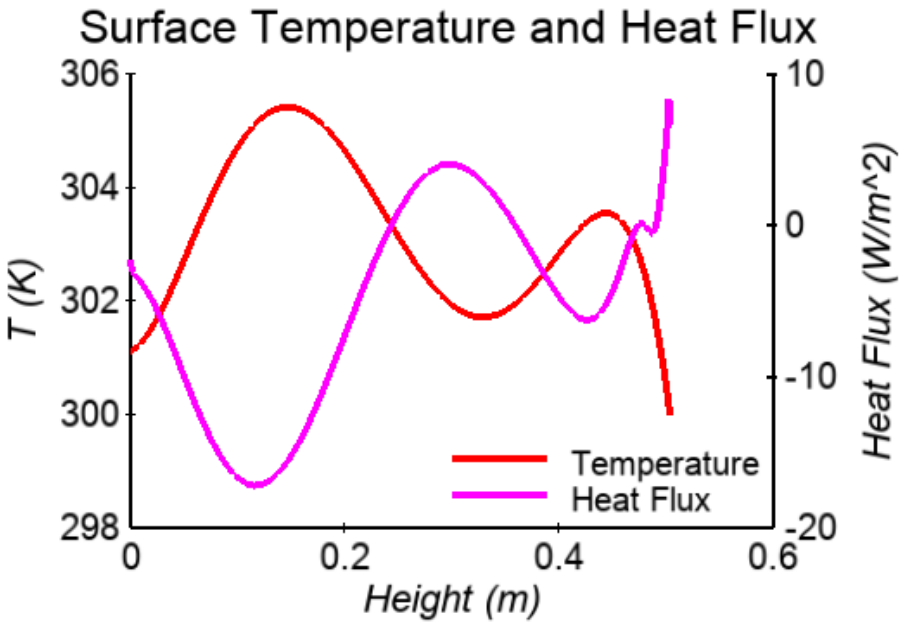
Is there a better way?

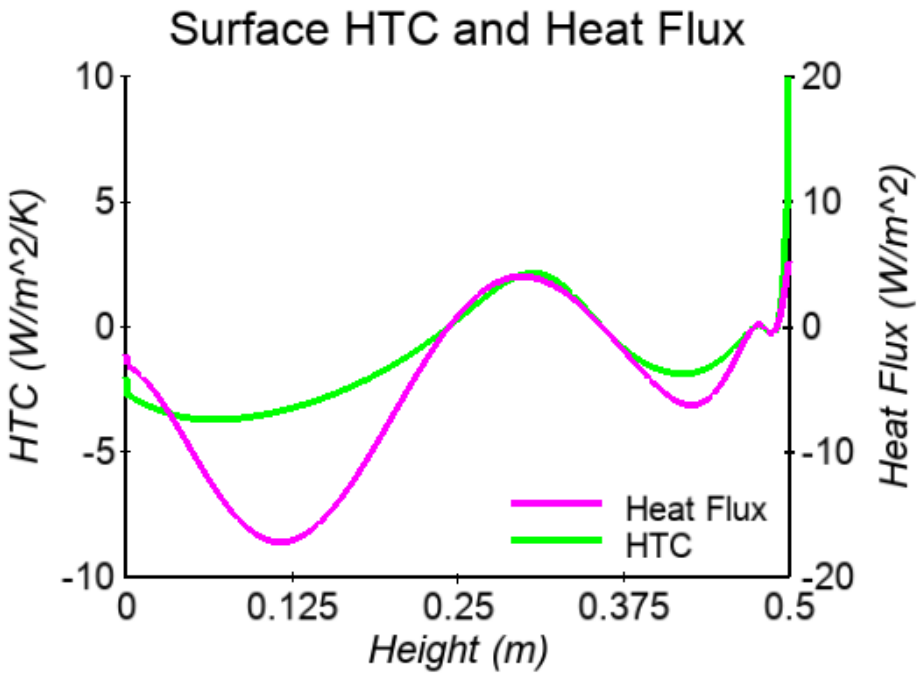
- It seems like I’m shoehorning in additional physics via surrogate models when we should be using a multi-physics package.

- Is there a use-case for using surrogate models in this way?
- Should the temperature and HTC distributions be decomposed differently?
  - Radial basis functions?
- What form should the surrogate model take?
  - PCE? Gaussian process?
- How big should the input space be?
  - Sensitivity study with FE model should answer this

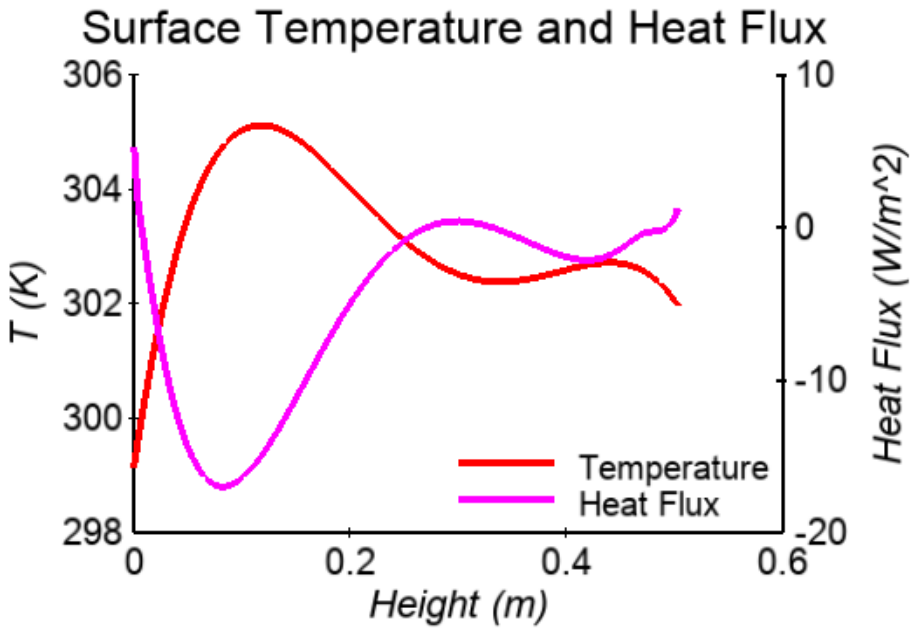
Appendix

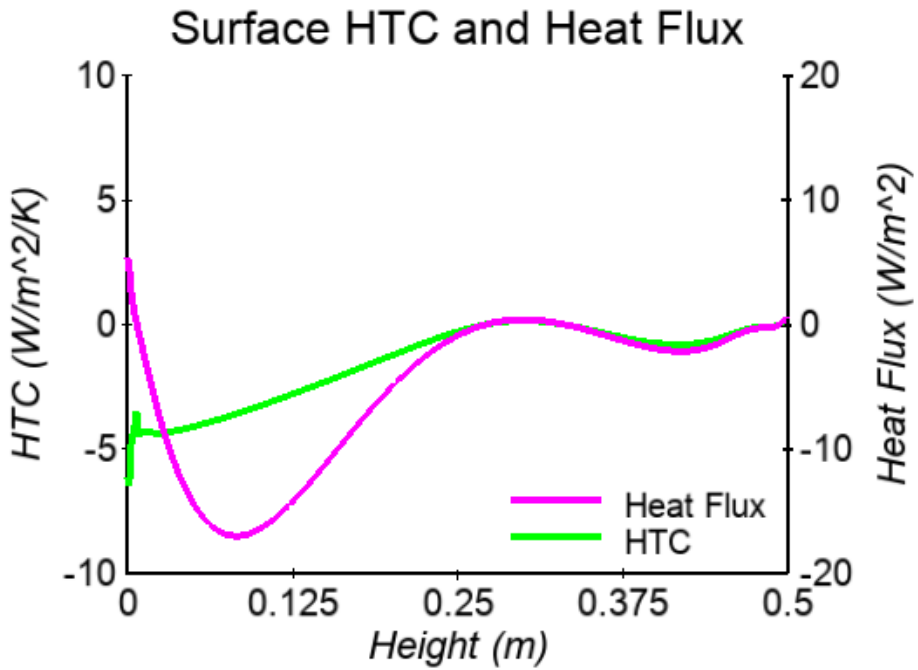
5th order PCE



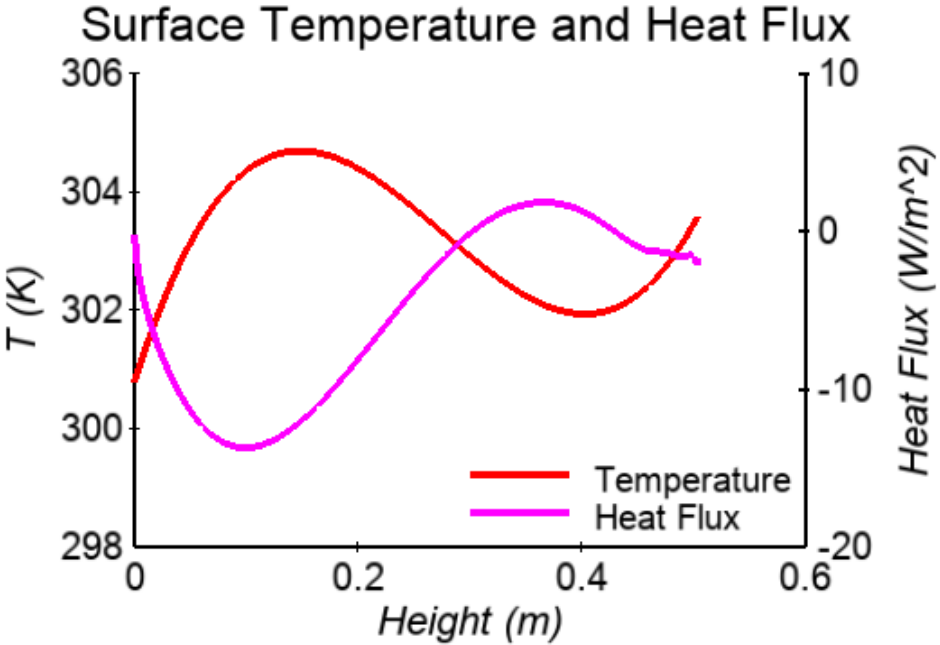


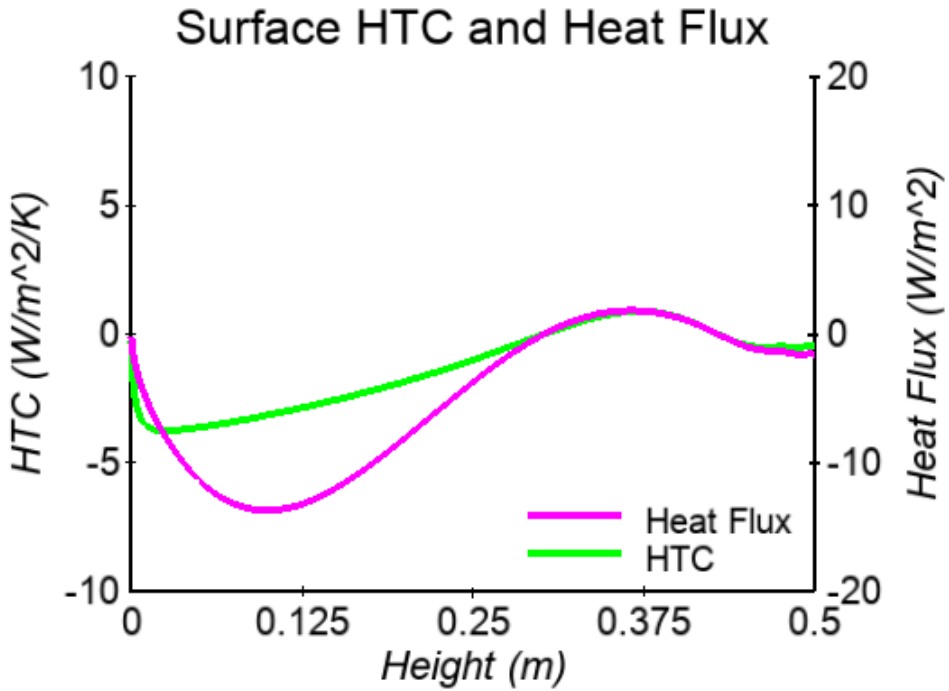
4th order PCE



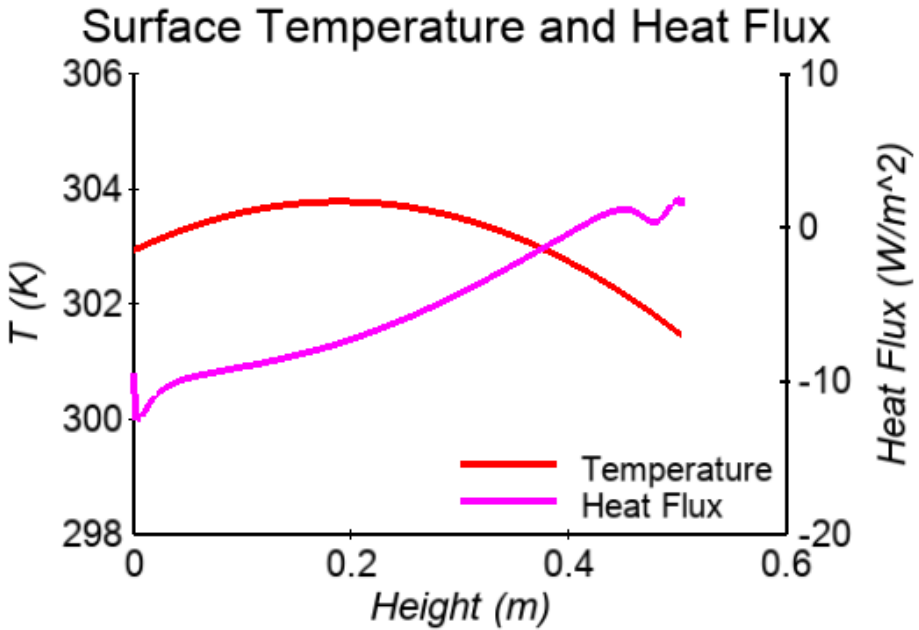


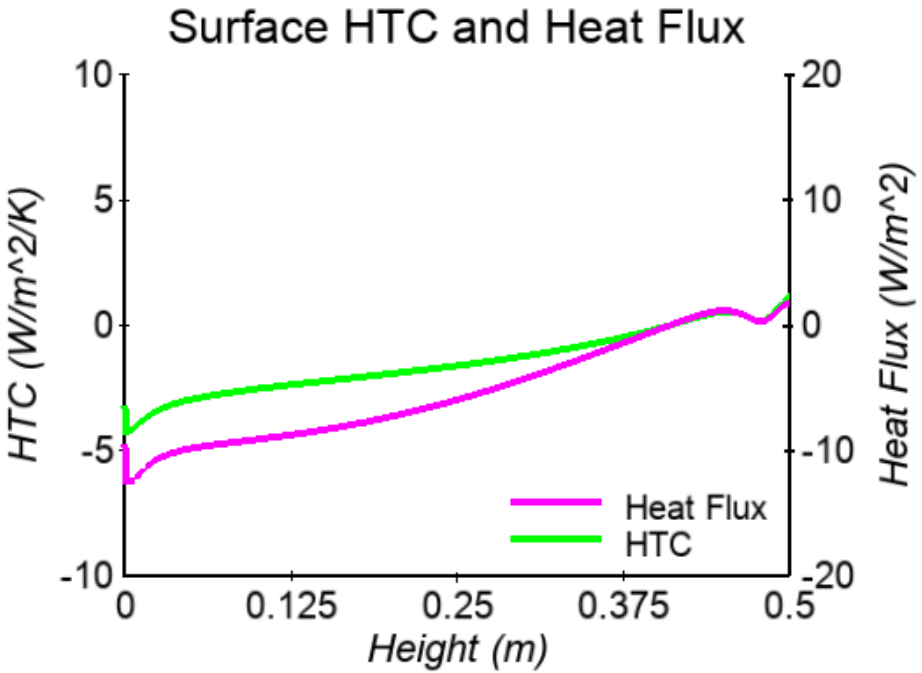
3rd order PCE



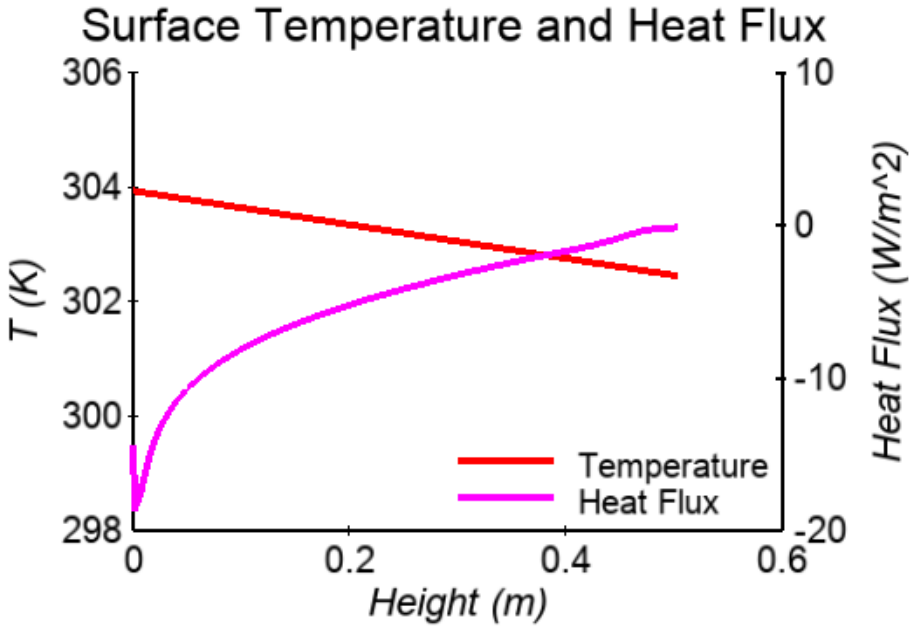


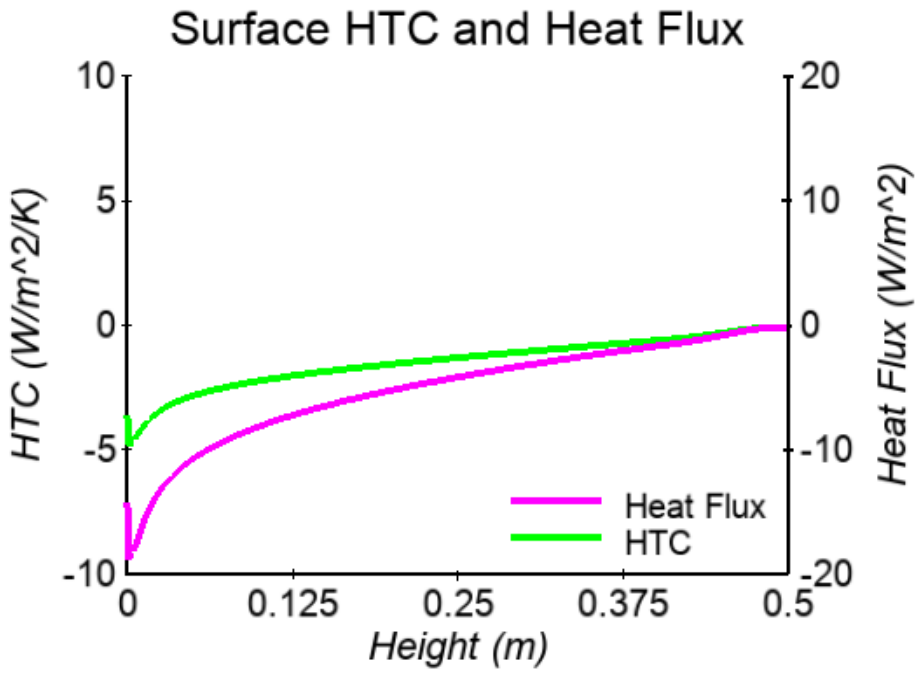
2nd order PCE





1st order PCE





0th order PCE